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Effect of impurities ordering in the electronic spectrum and conductivity of graphene

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ABSTRACT

By carrying out a computation in the Lifshitz tight-binding one-electron model, we obtain the energy spectrum and electrical conductance of graphene, in the presence of substitutional impurity atoms, thus assessing the influence of the latter. In the weak-scattering approximation, we study specific features of the electron energy spectrum in the gap region having width $\eta|\delta|$ and centered at the point $y\delta$, arising because of the ordering of substitutional impurity atoms on nodes of the crystal lattice. Here η is the parameter of ordering, δ is the difference of the scattering potentials of impurity atoms and carbon atoms, and y is the impurity concentration. It is shown that if the ordering parameter η is close to $\eta_{\max} = 2y$, $y < 1/2$, the plot of the density of electron states has peaks on the edges of the energy gap. Those peaks correspond to impurity levels. As the ordering parameter η decreases, the impurity levels split into the impurity bands. The regions of localization of electron impurity states, which arise at the edges of the spectrum and edges of the energy gap, are investigated.

1. Introduction

Most studies of the energy spectrum of graphene are based on the density functional theory [1] and are limited to numerical calculations, with the undoubted merit of showing the opening of a gap in the energy spectrum of graphene caused by the presence of an impurity [2–7]. It is obvious, though, that it is insufficient to restrict the analysis to numerical calculations only, in order to understand the nature of this effect. Instead, the influence of impurities on the energy spectrum and properties of graphene should be also described within a simple, but adequate model presenting the exact analytical solutions.

In the Lifshitz tight-binding one-electron model, the theory of reconstruction of the spectrum of graphene caused by an increase in the concentration of point impurities was developed in works [8–11]. Moreover, the possibility of the metal-dielectric transition in such system was predicted. Results of the analytical consideration of a reconstruction of the spectrum were confirmed with the help of a numerical experiment. It allowed one to verify the existence of a quasigap filled by localized states and showed its dominant role in the localization of the scattering by pairs and triples of impurity centers.

The numerical calculations within the Kubo–Greenwood quantum-mechanical formalism in the Lifshitz tight-binding one-electron model were performed in [12,13] to study the influence of impurity atoms or atoms adsorbed on the surface on the electronic structure and electrical conductance of graphene. In those works, the method of reduction of the Hamiltonian to the three-diagonal form was developed to study the influence of completely ordered impurity atoms on the energy spectrum and electrical conductance of graphene in the ballistic and diffusive modes of conductance. In work [13] in the Lifshitz tight-binding one-electron model, it was found that the gap 0.45 eV in width appears in the energy spectrum of electrons of graphene deposited on a potassium substrate. There, it was assumed that the appearance of this gap is associated with a change in the symmetry of the crystal. This assumption was corroborated in works [15–17]. Within the Lifshitz tight-binding one-electron model, the influence of the ordering of impurities on the energy spectrum and electrical conductance of graphene was considered in work [18]. It was established that the ordering of substitutional atoms on nodes of the crystal lattice [also] causes the appearance of a gap $\eta|\delta|$ in width in the energy spectrum of graphene centered at the point $y\delta$, where η is the ordering pa-

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